

Bis[4-(2-pyridylmethyleneamino)-phenyl] ether

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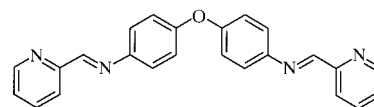
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The title compound, $C_{24}H_{18}N_4O$, is a bis-bidentate Schiff base ligand exhibiting pseudo- C_2 symmetry. The molecule is twisted about the central ether linkage and exhibits an imine E configuration. In the crystal, the molecules are linked by weak intermolecular $C-H \cdots N$ hydrogen bonds.

Comment

The processes by which transition metals and ligands spontaneously react to form a wide diversity of three-dimensional structural motifs are themes of intense current interest. The design of building blocks for self-assembly processes is the starting point for achieving new three-dimensional structures (Williams *et al.*, 1992; Lehn, 1995; Constable, 1996). Bis[4-(2-pyridylmethyleneamino)phenyl] ether, (I), is one such compound designed as a multidentate ligand for coordination with transition metals. Such ligands are sufficiently flexible to twist about the central O atom (or $-CH_2-$ bridge), but are not flexible enough to bend within themselves in order to coordinate all four donor atoms to the same metal atom. Cheng *et al.* (2000) and Tesouro Vallina & Stoeckli-Evans (1999) have shown that both triple and double binuclear helices can be

formed with (I). Recently, the structure of an Ag^I zigzag coordination polymer with (I) has been published (Tesouro Vallina & Stoeckli-Evans, 2001). Similar ligands with a $-CH_2-$ central linkage have already been shown to form double and triple binuclear helices (Hannon *et al.*, 1997; Hannon, Bunce *et al.*, 1999; Hannon, Painting & Alcock, 1999; Yoshida & Ichikawa, 1997; Yoshida *et al.*, 2000). Zacharias *et al.* (1995) studied the catalytic activity of some metal complexes of ligand (I).



(I)

Ligand (I) possesses pseudo-twofold symmetry, with the twofold axis running through the central O atom, and exhibits an imine E configuration (Fig. 1). The conformations of the two halves of the molecule differ considerably. One moiety, involving pyridine ring N4/C20–C24 and benzene ring C13–C18, is almost flat with a dihedral angle of $10.77(8)^\circ$ between the rings. In the second moiety, the pyridine ring N1/C1–C5 and benzene ring C7–C12 are inclined with respect to one another by $46.35(5)^\circ$. The pyridine–imine system is almost planar within the two moieties. The torsion angles N1–C5–C6–N2 and C7–N2–C6–C5 are $178.3(1)$ and $173.3(1)^\circ$, respectively, whereas torsion angles N3–C19–C20–N4 and C16–N3–C19–C20 are $171.0(1)$ and $-177.7(1)^\circ$, respectively. This is consistent with the presence of a π -conjugated system, only interrupted by the central O atom, although bond-length alternation is always observed [the average $C=N$ bond distance of $1.263(1)^\circ$ is indicative of double-bond character]. These characteristics are in agreement with similar structures (Orr *et al.*, 1992; Drew *et al.*, 1995).

In the crystal packing (Fig. 2), the pyridine N atoms are involved in weak intermolecular $C-H \cdots N$ interactions with symmetry-related molecules. The shortest interactions are found for $C18 \cdots N4^i$ and $C21 \cdots N1^{ii}$ with distances of $3.527(2)$ and $3.405(2) \text{ \AA}$, respectively. The more planar moieties of symmetry-related molecules are also considerably overlapped. A separation of *ca* 3.75 \AA was found between the best plane

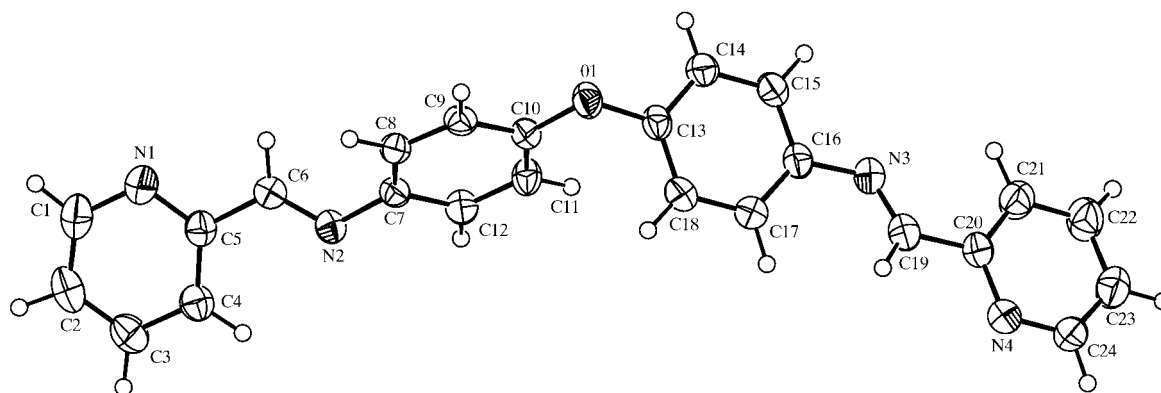


Figure 1

The structure of (I) showing the numbering scheme and displacement ellipsoids at the 50% probability level.

through the benzene ring (C13–C18) and the pyridine ring (N4/C20–C24; symmetry code: $2 - x, -y, 2 - z$), indicating weak π -stacking in the crystal.

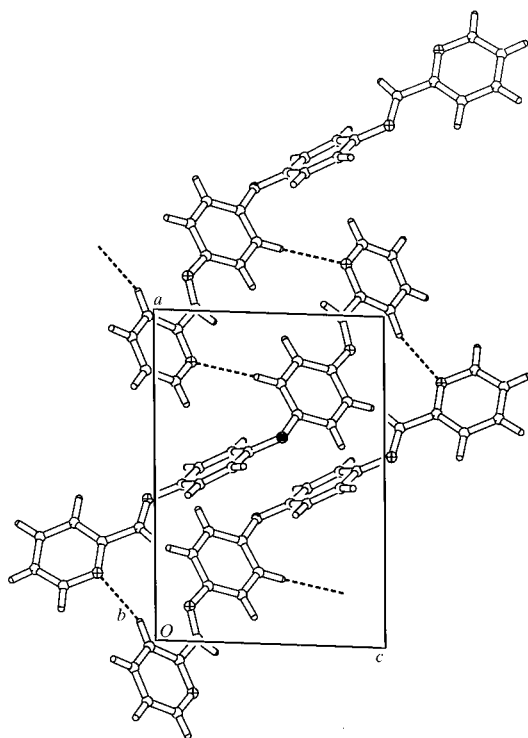


Figure 2
The crystal packing of (I) showing the C–H...N interactions as dotted lines.

Experimental

Ligand (I) was prepared by the Schiff base condensation of bis(4-aminophenyl) ether and 2-pyridinecarbaldehyde (Tesouro Vallina & Stoeckli-Evans, 1999; Cheng *et al.*, 2000). X-ray quality crystals were obtained from a CH_2Cl_2 solution layered with hexane at room temperature.

Crystal data

$\text{C}_{24}\text{H}_{18}\text{N}_4\text{O}$	$D_x = 1.291 \text{ Mg m}^{-3}$
$M_r = 378.42$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 5000 reflections
$a = 12.3403 (8) \text{ \AA}$	$\theta = 1.99\text{--}25.89^\circ$
$b = 18.3849 (17) \text{ \AA}$	$\mu = 0.082 \text{ mm}^{-1}$
$c = 8.5868 (6) \text{ \AA}$	$T = 153 (2) \text{ K}$
$\beta = 91.958 (8)^\circ$	Block, yellow
$V = 1947.0 (3) \text{ \AA}^3$	$0.55 \times 0.50 \times 0.35 \text{ mm}$
$Z = 4$	

Table 1

Hydrogen-bonding geometry (\AA , $^\circ$).

$D\text{--}H\cdots A$	$D\text{--}H$	$H\cdots A$	$D\cdots A$	$D\text{--}H\cdots A$
$\text{C18--H18}\cdots\text{N4}^i$	0.966 (17)	2.575 (17)	3.5265 (18)	168.1 (13)
$\text{C21--H21}\cdots\text{N1}^{ii}$	1.010 (16)	2.550 (17)	3.4046 (19)	142.2 (12)

Symmetry codes: (i) $2 - x, -y, 1 - z$; (ii) $1 - x, -y, 1 - z$.

Data collection

Stoe IPDS diffractometer	$R_{\text{int}} = 0.032$
φ oscillation scans	$\theta_{\text{max}} = 25.89^\circ$
14238 measured reflections	$h = -14 \rightarrow 15$
3716 independent reflections	$k = -22 \rightarrow 22$
2904 reflections with $I > 2\sigma(I)$	$l = -10 \rightarrow 10$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0555P)^2 + 0.1419P]$
$R[F^2 > 2\sigma(F^2)] = 0.035$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.094$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 1.015$	$\Delta\rho_{\text{max}} = 0.16 \text{ e \AA}^{-3}$
3716 reflections	$\Delta\rho_{\text{min}} = -0.13 \text{ e \AA}^{-3}$
334 parameters	
All H-atom parameters refined	

The H atoms were located from Fourier difference maps and refined isotropically [$\text{C--H} = 0.93 (2)\text{--}1.02 (2) \text{ \AA}$].

Data collection: *EXPOSE* (Stoe & Cie, 2000); cell refinement: *CELL* (Stoe & Cie, 2000); data reduction: *INTEGRATE* (Stoe & Cie, 2000); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON99* (Spek, 1990); software used to prepare material for publication: *SHELXL97*.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: JZ1445). Services for accessing these data are described at the back of the journal.

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